

Structure of ^{78}Ni from first principles computations

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Doubly magic nuclei have a simple structure and are the cornerstones for entire regions of the nuclear chart. Theoretical insights into the supposedly doubly magic ^{78}Ni and its neighbors are challenging because of the extreme neutron-to-proton ratio and the proximity of the continuum. We predict the $J^\pi = 2_1^+$ state in ^{78}Ni from a correlation with the $J^\pi = 2_1^+$ state in ^{48}Ca using chiral nucleon-nucleon and three-nucleon interactions. Our results confirm that ^{78}Ni is doubly magic, and the predicted low-lying states of $^{79,80}\text{Ni}$ open the way for shell-model studies of many more rare isotopes.

Introduction – Doubly magic nuclei, i.e. nuclei with closed proton and neutron shells, play a most important role in nuclear physics [1]. They are more strongly bound than their neighbors, exhibit simple regular patterns, and are the cornerstones for our understanding of nuclear structure in entire regions of the Segré chart. In recent years, experiments and theory have made considerable progress in uncovering the evolution of shell structure in rare isotopes of oxygen [2–11], calcium [12–18], and tin [19–21].

The supposedly doubly magic nucleus ^{78}Ni (with neutron number 50 and proton number 28) has been the focus of considerable experimental and theoretical efforts [22–28]. This nucleus is also of astrophysical relevance because it is in the region of the r -process path. Reliable theoretical predictions for ^{78}Ni and its neighbors are challenging [29, 30], because of the extreme neutron-to-proton ratio and the proximity to the neutron dripline. The large isospin brings to the fore smaller aspects of the nuclear interaction that are poorly constrained in β stable nuclei, while for weakly bound and unbound nuclear states it is necessary to include coupling to the particle continuum. We address these challenges as follows: We employ a set of interactions [31, 32] from chiral effective field theory (EFT) [33–35]. These interactions consist of nucleon-nucleon (NN) and three-nucleon forces (3NFs) [36, 37]. They reproduce properties of nuclei with mass numbers $A = 2, 3, 4$ nuclei well, but differ in binding energies, radii, and spectra of medium-mass nuclei [38]. We include continuum physics by employing the Berggren basis [39–41] which treats bound-, resonant-, and non-resonant scattering states on equal footing. The Berggren basis has been extensively used in the Gamow-shell-model and coupled-cluster computations of weakly bound and unbound nuclear states, see for example [42–44]. Finally, using these ingredients we solve for the structure of ^{78}Ni and its neighbors using coupled-cluster theory [45–54], see Refs. [55, 56] for recent reviews. For the computation of $J^\pi = 2_1^+$ excited states in ^{48}Ca and ^{78}Ni we use an implementation of the equation-of-motion (EOM) coupled-cluster method that properly accounts for two-particle-two-hole ($2p\text{-}2h$) exci-

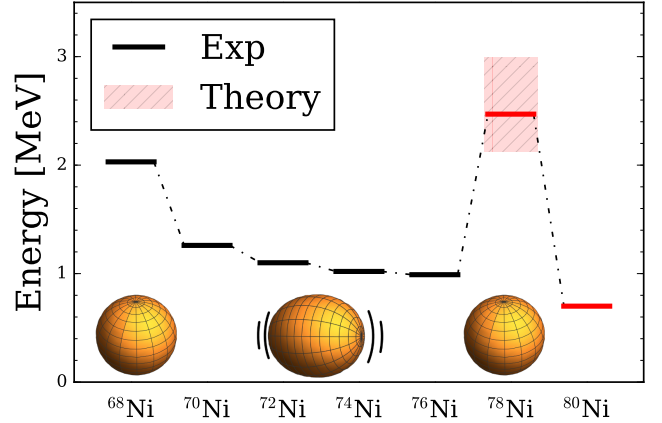


FIG. 1. (Color online) Energy of the 2_1^+ state in neutron-rich nickel isotopes for $^{68-76}\text{Ni}$ from data (black horizontal lines) and for $^{78,80}\text{Ni}$ from first-principles computations (red horizontal lines) based on the chiral interaction “1.8/2.0 (EM)” of Ref. [31]. The red shaded area for ^{78}Ni shows the predicted range for the 2_1^+ state based on a correlation between the 2_1^+ in ^{48}Ca and ^{78}Ni using a family of chiral interactions (see text and Fig. 2 for details).

tations.

As a key indicator of the ^{78}Ni structure, we focus on the energy of the first excited $J^\pi = 2_1^+$ state. This 2_1^+ state is at about 1 MeV of excitation energy in $^{70,72,74,76}\text{Ni}$, reflecting a softness regarding (a collective) quadrupole vibration. In contrast to these semi magic nuclei, the nucleus ^{68}Ni exhibits a soft subshell closure (at neutron number 40) [57, 58], and its 2_1^+ state is at about 2 MeV of excitation energy. This situation is illustrated in Fig. 1, with experimentally known 2_1^+ levels shown as black bars and the computed energies of the 2_1^+ states in $^{78,80}\text{Ni}$ from this Letter. For ^{78}Ni the red shaded area gives the predicted range for the 2_1^+ state obtained by correlating relevant observables; details are given below. The predicted range for the 2_1^+ state in ^{78}Ni is considerably higher than for its neighbors – indicating that this nucleus is doubly magic. This is the main result of this Letter. The red bar marks the result obtained with the

interaction “1.8/2.0(EM)” from Ref. [31], which is singled out because it accurately reproduces the binding energy of ^{78}Ni , as well as the nuclei ^4He , ^{16}O , and $^{40,48}\text{Ca}$.

This Letter is organized as follows. We briefly summarize the Hamiltonian and model-spaces that are input to the calculations of neutron-rich nickel isotopes. We discuss an implementation of three-particle-three-hole corrections to coupled-cluster computations of excited states. Using these theoretical ingredients we compute the first 2_1^+ state in the doubly magic ^{48}Ca and in ^{78}Ni from a family of chiral NN and 3NFs . From an observed correlation between the energies of the 2_1^+ states in ^{48}Ca and ^{78}Ni we obtain a range for the latter. We discuss the relevance of $2p$ - $2h$ excitations in this state. We also give predictions for other low-lying states in ^{78}Ni . Finally we focus on the neighbors of ^{78}Ni and present predictions for low-lying states in $^{77,79,80}\text{Ni}$.

Hamiltonian and model-space – Our coupled-cluster calculations start from the intrinsic Hamiltonian

$$\hat{H} = \sum_{i < j} \left(\frac{(\mathbf{p}_i - \mathbf{p}_j)^2}{2mA} + \hat{V}_{NN}^{(i,j)} \right) + \sum_{i < j < k} \hat{V}_{3N}^{(i,j,k)}. \quad (1)$$

We compute the Hamiltonian (1) using interactions from Refs. [31, 32]. The interactions of Ref. [31] are based on similarity-renormalization-group (SRG) [59] transformations of NN interactions from chiral EFT augmented with leading 3NFs from chiral EFT. Here, the low-energy constants of the 3NFs are adjusted to data from nuclei with mass numbers $A = 3, 4$. These interactions yield saturation points for nuclear matter around the empirical value [31], and they yield radii and binding energies in calcium isotopes scattered around data [38]. The interaction NNLO_{sat} of Ref. [32] by construction yields accurate radii and binding energies in light nuclei and isotopes of oxygen. It extrapolates well to calcium isotopes [38] and ^{56}Ni [60], and within uncertainties reproduces the empirical saturation point in symmetric nuclear matter. We employ these interactions to study systematic sensitivities because a full-fledged propagation of uncertainties is not yet possible [61].

We use a Hartree-Fock basis constructed from a harmonic oscillator basis of up to 15 major oscillator shells. To compute weakly bound and unbound states in ^{79}Ni we construct a Gamow-Hartree-Fock basis [44, 62] by including a Berggren basis for relevant partial waves and follow Ref. [60] for inclusion of 3NFs . For ^{48}Ca we use the same model-spaces that were employed in Ref. [38], while for the neutron-rich nickel isotopes we perform the calculations at the oscillator frequency $\hbar\omega = 16$ MeV which yields the minimum in energy for the largest model-space that we consider. We use the normal-ordered two-body approximation [63–65] for the 3NF with the additional three-body energy cut $E_{3\text{max}} = N_1 + N_2 + N_3 \leq 16$. Here $N_i = 2n_i + l_i$ refers to the oscillator shell of the i^{th} particle.

Method – We employ the coupled-cluster singles-doubles (CCSD) approximation in an angular momentum coupled representation in the computation of the similarity-transformed Hamiltonian \bar{H} (see Refs. [56, 66] for details). We include triple excitations perturbatively using the Λ -CCSD(T) method [67] for the computation of the ground-state energy. The excited 2_1^+ state is computed with the EOM coupled-cluster method in the EOM-CCSD [68] and EOM-CCSD(T) approximations [69]. EOM-CCSD has been shown to be accurate for states that are dominated by $1p$ - $1h$ excitations [55]. In this Letter we go beyond the standard EOM-CCSD approach and include corrections from $3p$ - $3h$ excitations perturbatively using the EOM-CCSD(T) approach. EOM-CCSD(T) capture the dominant $2p$ - $2h$ excitations in the computation of the 2_1^+ state in ^{48}Ca and ^{78}Ni . This method is a generalization of the Λ -CCSD(T) approach for the ground-state energy and requires the solution of both the left and right EOM-CCSD eigenvalue problem, and with a non-iterative $3p$ - $3h$ correction computed perturbatively. We note that the computational cost is considerably larger than for Λ -CCSD(T) since we are considering a non-scalar excitation. In quantum chemistry applications, EOM-CCSD(T) is an economical and accurate correction to EOM-CCSD [70]. Excited states in neighboring nuclei $^{77,79,80}\text{Ni}$ are computed as generalized mp - nh excited states [66, 71, 72] of \bar{H} . Details of this approach are presented in the review [56] and in the supplementary material of Ref. [38].

Results – To probe the quality of the EOM-CCSD(T) approximation, and for a comparison with data, we also compute the 2_1^+ excited state in ^{48}Ca . For the computation of the 2_1^+ state in ^{78}Ni , we employ the same interactions but choose lower model space frequencies to stabilize the ground-state energies.

Figure 2 shows that the excitation energy of the 2_1^+ state in ^{48}Ca and ^{78}Ni are strongly correlated. The error bars on the individual data points estimate uncertainties from the method and model-space truncation. We estimate the model-space uncertainty from enlarging the model space from $N = 12$ to $N = 14$ which is less than 200 keV for all employed interactions. For the method we include 10% of the triples correlation energy as an uncertainty estimate. We take the average from all interactions and give a combined uncertainty on the 2_1^+ state in ^{48}Ca and ^{78}Ni . A linear fit to the data points, and an encompassing diagonal uncertainty band is also shown. The thin horizontal line marks the known energy of the 2_1^+ state in ^{48}Ca , and its intersection with the diagonal band projects out our theoretical estimate $2.1 \text{ MeV} \lesssim E(2_1^+) \lesssim 3.1 \text{ MeV}$ for the energy of the 2_1^+ state in ^{78}Ni . This band is also shown in Fig. 1. We note that two of the five employed interactions reproduce the energy of the 2_1^+ state in ^{48}Ca within uncertainties. The interaction NNLO_{sat} , which accurately reproduces charge radii in ^{48}Ca , yields an excitation energy that is

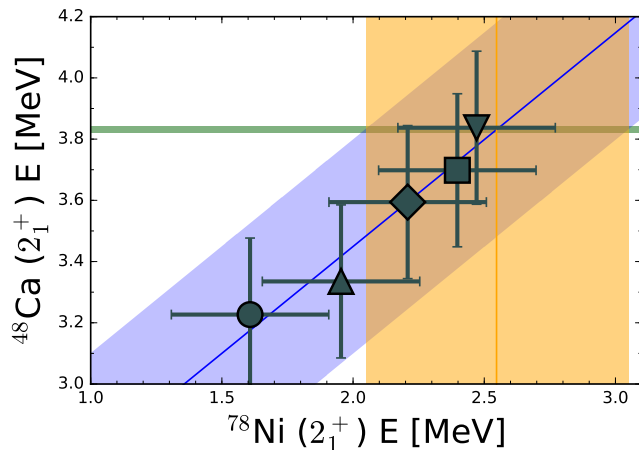


FIG. 2. (Color online) Correlation between the energies of the 2_1^+ excited state in ^{48}Ca and ^{78}Ni , obtained from the interactions NNLO_{sat} (circle), “2.0/2.0 (PWA)” (square), “2.0/2.0 (EM)” (diamond), “2.2/2.0 (EM)” (triangle up), and “1.8/2.0 (EM)” (triangle down). The error bars estimate uncertainties from enlarging the model space from $N = 12$ to $N = 14$. The thin horizontal line marks the known energy of the 2_1^+ state in ^{48}Ca .

too low. We also note that the origin of the correlation between the 2_1^+ states in ^{48}Ca and ^{78}Ni depicted in Fig. 2 is not understood theoretically. While several such correlations have been reported (and exploited) in the literature, see, e.g., Refs. [38, 73, 74], only few have been understood [75]. The spectroscopy of ^{78}Ni was recently measured at RIBF, RIKEN [76], and it will be interesting to compare our theoretical result with data.

For ^{78}Ni , the convergence of the ground-state energy with respect to the size of the model space is slow for most of the employed interactions, and we are only able to achieve convergence for the softest interaction “1.8/2.0 (EM)” of Ref. [31]. For this interaction the computed binding energy is 637(4) MeV which agrees with the value 641 MeV extracted from systematic trends. The $E_{3\text{max}}$ truncation used for the 3NF is the dominant uncertainty, and the estimated error of 4 MeV comes from increasing $E_{3\text{max}}$ from 14 to 16. We note that the convergence is improved for energy differences. Figure 3 shows the convergence of the energy of the 2_1^+ state in ^{48}Ca and ^{78}Ni with increasing size of the model space, obtained for the interaction “1.8/2.0 (EM)”. The convergence is qualitatively similar for the other interactions, and the difference between the $N = 12$ and $N = 14$ spaces entered the uncertainties presented in Fig. 2.

We note that the interaction “1.8/2.0 (EM)” describes of the 2_1^+ state in ^{48}Ca and the binding energies for a variety of nuclei remarkably well. For example, the computed binding energies for ^4He , ^{16}O and $^{40,48}\text{Ca}$ are 28.2 MeV, 128 MeV, 348 MeV, and 419 MeV, respectively; they are close to the corresponding experimental binding energies

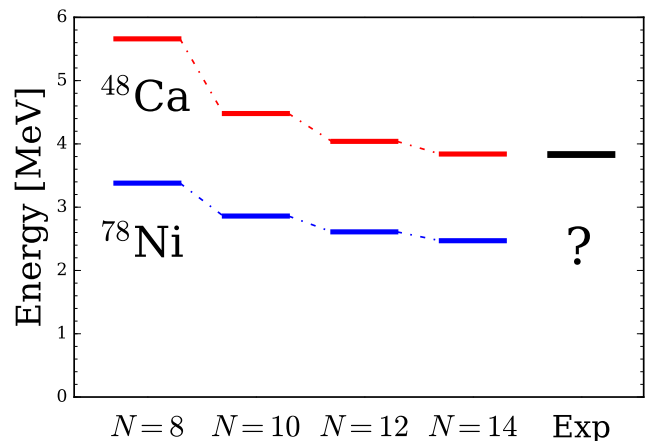


FIG. 3. (Color online) Convergence of the first 2_1^+ excited state of ^{48}Ca and ^{78}Ni with increasing model-space size and compared to data for the interaction “1.8/2.0 (EM)” of Ref. [31].

of 28.2 MeV, 128 MeV, 342 MeV, and 416 MeV.

Let us discuss the effect of $2p\text{-}2h$ excitations in the 2_1^+ excited state of ^{48}Ca and ^{78}Ni . Table I shows results for this state using the EOM-CCS, EOM-CCSD and EOM-CCSD(T) approximations for the interactions used in this work. We find that the inclusion of perturbative $3p\text{-}3h$ excitations in EOM-CCSD(T) reduces the excitation energy by 1-2 MeV for all interactions when compared to the corresponding EOM-CCSD results. The triples corrections for the 2_1^+ state in both ^{48}Ca and in ^{78}Ni amounts to about 20% of the EOM-CCSD correlation energy (defined as the difference between the EOM-CCS and EOM-CCSD excitation energies). We note that the role of $3p\text{-}3h$ excitations in the computation of the 2_1^+ state in both ^{48}Ca and in ^{78}Ni is considerably larger than the role of $3p\text{-}3h$ excitations in the ground-state. For the ground-state of closed (sub-)shell nuclei the triples correlation energy typically amounts to about 10% of the CCSD correlation energy, see Ref. [77] for an example.

| Interaction | ^{48}Ca | | | ^{78}Ni | | |
|----------------------------|------------------|-------|-------|------------------|-------|-------|
| | 1p-1h | 2p-2h | 3p-3h | 1p-1h | 2p-2h | 3p-3h |
| 1.8/2.0 (EM) | 10.5 | 4.9 | 3.8 | 8.5 | 3.5 | 2.5 |
| 2.0/2.0 (EM) | 11.3 | 4.9 | 3.6 | 9.1 | 3.4 | 2.2 |
| 2.2/2.0 (EM) | 12.0 | 4.8 | 3.3 | 9.5 | 3.4 | 2.0 |
| 2.0/2.0 (PWA) | 12.0 | 5.2 | 3.7 | 9.8 | 3.8 | 2.4 |
| NNLO_{sat} | 14.8 | 5.3 | 3.2 | 12.2 | 3.8 | 1.6 |

TABLE I. Results for the excitation energy (in MeV) of the 2_1^+ state in ^{48}Ca and ^{78}Ni computed in the EOM-CCS (denoted by 1p-1h), EOM-CCSD (denoted by 2p-2h) and EOM-CCSD(T) (denoted by 3p-3h) approximations. The interactions labeled (EM) and (PWA) are taken from Ref. [31] and NNLO_{sat} is from Ref. [32].

Our analysis shows that $2p\text{-}2h$ excitations are signif-

icant for the 2_1^+ state in ^{48}Ca and ^{78}Ni , and that a precise description of this state therefore requires EOM-CCSD(T). This finding is somewhat surprising, because the collective 2_1^+ state is usually thought of as a coherent superposition of $1p$ - $1h$ excitations [78]. However, a simple shell-model argument suggests that $2p$ - $2h$ excitations should yield significant corrections. In the doubly-magic ^{48}Ca for instance, no $1p$ - $1h$ excitations of protons near the Fermi surface can generate a 2^+ state, as one needs at least $2p$ - $2h$ excitations from the sd shell to the pf shell to yield a 2^+ state. Following the same reasoning, a computation of the electric quadrupole transition in ^{48}Ca will have significant $2p$ - $2h$ contributions since this observable measures mostly the excitations of protons. Similarly, we find that for ^{78}Ni $2p$ - $2h$ excitations of neutrons near the Fermi surface have significant contributions to the low-lying 2_1^+ state. In the naive shell-model picture the $g_{9/2}$ orbital is the last filled neutron shell with $s_{1/2}, d_{5/2}, d_{3/2}, g_{7/2}$ shells being the next unoccupied orbitals closest to the Fermi surface. A 2^+ state near the Fermi surface can be generated via $1p$ - $1h$ excitations of neutrons from the $g_{9/2}$ to the $d_{5/2}, g_{7/2}$ orbitals, but $2p$ - $2h$ excitations are necessary to utilize the low-lying $s_{1/2}$ and $d_{3/2}$ orbitals. As shown in Tab. I the effect of $2p$ - $2h$ excitations from the $g_{9/2}$ to the $s_{1/2}$ and $d_{3/2}$ orbitals is significant in the 2^+ state of ^{78}Ni . As we will see below the $1/2^+$ state is actually the lowest state in ^{79}Ni .

Shell closures manifest themselves in several observables. Besides the energy of the 2_1^+ state, separation energies also yield valuable information. For the computation of other low-lying states in ^{78}Ni and in the neighboring nuclei $^{77,79,80}\text{Ni}$, we limit ourselves to the “1.8/2.0 (EM)” interaction because this interaction yields converged results with respect to the model space and accurate binding energies from ^4He to ^{16}O to ^{48}Ca to ^{78}Ni . For ^{79}Ni , we employed a Berggren basis for the $s_{1/2}, d_{5/2}$ and $d_{3/2}$ partial waves because of the proximity of the continuum. For the $g_{7/2}$ partial wave we use the harmonic-oscillator basis, because the large centrifugal barrier reduces the impact of the coupling to the continuum. The resulting spectra are shown in Fig. 4 relative to the ground-state energy of ^{78}Ni . For ^{78}Ni we predict low-lying $1_1^+, 3_1^+, 4_1^+$ excited states all below the neutron-emission threshold. The ratio of the excited 4_1^+ state with the 2_1^+ state is 1.2, which is consistent with ^{78}Ni being a doubly magic nucleus. Due to the high computational cost the $1_1^+, 3_1^+, 4_1^+$ excited states in ^{78}Ni were computed with $N = 12$; the triples correlation energy for the 4_1^+ state was well converged for $N = 10$. The theoretical result for the neutron-separation energies in $^{78,79}\text{Ni}$ are $S_n \approx 4.5$ MeV and $S_n \approx 1$ MeV, respectively, which are consistent with 5450(950) keV and 1650(1130) keV from systematics [79]. For ^{79}Ni we find that the inclusion of the continuum impacts the level ordering and lowers the $1/2^+$ state by about 1 MeV, the $5/2^+$ state by about 0.5 MeV, and the unbound $3/2^+$ state by about 0.7 MeV, as compared to

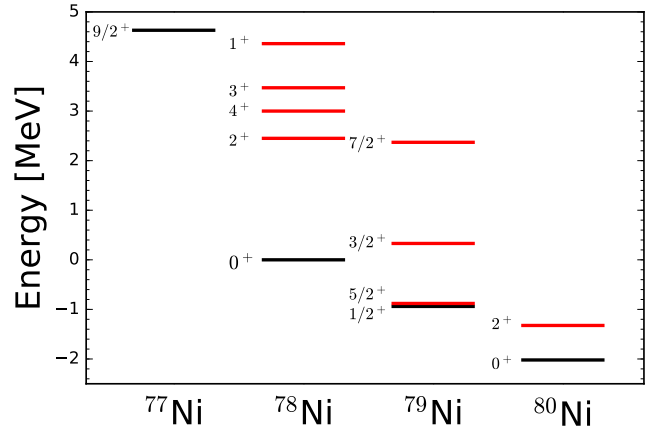


FIG. 4. (Color online) Low-lying states in $^{77-80}\text{Ni}$ with respect to the ground-state of ^{78}Ni computed with the interaction “1.8/2.0 (EM)” of Ref. [31]. The ground states are shown in black, while excited states are shown in red.

a calculation using harmonic oscillator functions only.

The $1/2^+$ ground-state of ^{79}Ni is quasi-degenerate with the $5/2^+$ state. This finding mirrors the results of Refs. [14, 60, 80], where the inclusion of continuum effects also impacted the energies and level ordering of unbound states in the neutron-rich calcium isotopes $^{53,55,61}\text{Ca}$. The ground-state of ^{80}Ni is bound by 2 MeV with respect to ^{78}Ni , thereby setting the neutron dripline beyond ^{80}Ni . This is consistent with mean-field surveys [81]. The two-neutron separation $S_{2n}(^{80}\text{Ni}) \approx 2$ MeV is significantly smaller than the estimate $S_{2n}(^{78}\text{Ni}) = 8660(950)$ keV [79] – consistent with expectations for a doubly magic nucleus. The 2_1^+ state in ^{80}Ni is computed to be 0.7 MeV above its ground state. The combined results of this study – a relatively high-lying 2_1^+ state in ^{78}Ni , the marked difference of neutron-separation energies between ^{79}Ni and ^{78}Ni , and of two-neutron separation energies between ^{80}Ni and ^{78}Ni , respectively, indicate the strength of the shell closure at neutron number 50.

Conclusions – We presented first-principles computations of the structure of ^{78}Ni and its neighbors. Correlating the 2_1^+ energies in ^{78}Ni and ^{48}Ca leads to the prediction $2.1 \text{ MeV} \lesssim E(2_1^+) \lesssim 3.1 \text{ MeV}$ for the energy of the 2_1^+ state in ^{78}Ni . Neutron separation energies and two-neutron separation energies confirm the picture of the shell closure at neutron number 50, and the theoretical results put the neutron dripline beyond ^{80}Ni . We also made predictions for low-lying states in $^{77,78,79,80}\text{Ni}$ that can be confronted by experiment. As a useful theoretical tool, a relatively soft chiral interaction emerged as being in good agreement with binding energies and low-lying excitations from ^4He , to ^{16}O , to $^{40,48}\text{Ca}$ to ^{78}Ni . This study paves the way to theoretical predictions in heavy rare isotopes.

We thank Kai Hebeler for providing us with matrix

elements in Jacobi coordinates for the three-nucleon interaction at next-to-next-to-leading order. This work was supported by the Office of Nuclear Physics, U.S. Department of Energy, under grants DE-FG02-96ER40963, DE-SC0008499 (NUCLEI SciDAC collaboration), and the Field Work Proposal ERKBP57 at Oak Ridge National Laboratory (ORNL). Computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility located at ORNL, which is supported by the Office of Science of the Department of Energy under Contract No. DE-AC05-00OR22725.

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